

The Quantum Liouville Equation for the Effective Action

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Abstract

Starting from the von Neumann equation, we construct the quantum evolution equation for the effective action for systems in mixed states. This allows us to find the hierarchy of equations which describe the time evolution of equal time correlators. The method is applied explicitly to a scalar theory with quartic self-interaction.

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Introduction

During the last years, great progress has been made in the study of statistical systems of quantized fields in thermal equilibrium. Many physically interesting quantities, however, are typically related to out-of equilibrium scenarios, like density fluctuations in the early universe, the radiation signature of hot quark-gluon matter or baryon number violating processes. The study of such quantities in systems which are not near to equilibrium requires a framework which is able to deal with mixed states characterized by general density matrices.

Although the Schrödinger equation already determines the exact evolution of initial density matrices and can be integrated to solve the problem of time evolution, it is of less use for practical purposes. What one is interested in and what is used to describe a physical system is not the density matrix but a number of observables derived from it. At first sight it may appear to be rather a matter of taste to study time evolution of observables instead of the density matrix, but there is also a profound physical reason to change the point of view. Time integration of the density matrix requires the exact knowledge of the initial state, which is not accessible since observation is usually restricted to only a small number data. Consequently, the description of a system requires apart from the knowledge of the exact motion of observables also a statistical assumption replacing the incomplete knowledge of the initial state.

In this letter we focus on the first step of the problem. We investigate on the exact counterpart of what the Schrödinger equation is for the density matrix: A quantum Liouville equation for the effective action which encodes in a compact form the time evolution of all equal time correlators being one basis of a complete set of observables.

Construction

The following construction will be formulated in the Schrödinger picture, that means operators are time independent and time evolution is contained in the density matrix. The resulting evolution equation, however, is independent of the picture chosen.

Starting point is the von Neumann equation for the density matrix operator,

$$i\partial_t\rho(t) = [H, \rho(t)], \quad (1)$$

with Hamiltonian H . It is a functional of the position operator $\Phi(\mathbf{x})$ and its canonical momentum operator $\Pi(\mathbf{x})$. In a given mixed state described by a density matrix $\rho(t)$, operator expectation values are given by the trace average

$$\langle\mathcal{O}\rangle_t = \text{tr}(\mathcal{O}\rho(t)), \quad (2)$$

where the hermitian density matrix is normalized to unity, $\text{tr}\rho(t) = 1$, which is consistent with unitary time evolution.

We introduce the generating functional of polynomials in momentum and position operators by

$$Z[j, k; t] = \langle D[j, k] \rangle_t = \text{tr}(D[j, k] \rho(t)) \quad (3)$$

with current operator

$$D[j, k] = \exp(ij \cdot \Phi + ik \cdot \Pi) \quad (4)$$

and shorthand notation $j \cdot \Phi := \int d^3x j(\mathbf{x}) \Phi(\mathbf{x})$.

Since neither position nor momentum operators explicitly depend on time, integration is done with respect to space only, and also there is no need to introduce time dependent currents. This is a very special feature of the Schrödinger picture where all the dynamics is hidden in the states and the density matrix. The definition breaks Lorentz invariance. However, it is broken anyway since in the Hamilton formulation the time direction (evolution direction) orthogonal to the time slice of quantisation plays a privileged rôle.

The current operator can be rewritten as

$$D[j, k] = \exp(ij \cdot \Phi) \exp(ik \cdot \Pi) \exp\left(\frac{i}{2} j \cdot k\right) = \exp(ik \cdot \Pi) \exp(ij \cdot \Phi) \exp\left(-\frac{i}{2} j \cdot k\right) \quad (5)$$

using the fundamental commutator $[\Phi(\mathbf{x}), \Pi(\mathbf{y})] = i\delta^3(\mathbf{x} - \mathbf{y})$ and the first non-trivial term in the Campbell-Baker-Hausdorff formula. From that representation, powers of position and momentum operators can be obtained by the functional differential operators,

$$\left(\frac{\delta}{i\delta j} - \frac{1}{2}k\right) D[j, k] = \Phi D[j, k], \quad \left(\frac{\delta}{i\delta k} + \frac{1}{2}j\right) D[j, k] = \Pi D[j, k], \quad (6)$$

or, equivalently, by acting from the left with

$$D[j, k] \left(\frac{\overleftarrow{\delta}}{i\delta j} + \frac{1}{2}k\right) = D[j, k] \Phi, \quad D[j, k] \left(\frac{\overleftarrow{\delta}}{i\delta k} - \frac{1}{2}j\right) = D[j, k] \Pi. \quad (7)$$

Polynomial operator expectation values $\mathcal{O}[\Phi, \Pi]$ can thus be cast by firstly constructing the operator with inverse order by reading it from the right to the left, secondly the replacements $\Phi \rightarrow (\delta/i\delta j - k/2)$ and $\Pi \rightarrow (\delta/i\delta k + j/2)$ in the inverse ordered operator, third acting with this expression on the generating functional, and finally letting $j, k \rightarrow 0$ afterwards. We note that the functional differential operator replacements have the negative commutator with respect to their field operator counterparts. We also note that if we used the representations $\Phi \rightarrow \delta/i\delta j$ and $\Pi \rightarrow \delta/i\delta k$ instead of those of Eq. (6), we get the symmetrically ordered operator polynomial.

Let us construct the time evolution of the generating functional. From its definition and the equation of motion for the density matrix, we get

$$\partial_t Z[j, k; t] = i \text{tr}(H[\Pi, \Phi] D[j, k] \rho(t)) - i \text{tr}(D[j, k] H[\Pi, \Phi] \rho(t)). \quad (8)$$

In view of the arguments given above, the Hamiltonian can now be replaced by a functional differential operator which can be drawn out of the trace. We get a Liouville equation for the generating functional

$$\partial_t Z[j, k; t] = L[j, k] Z[j, k; t] \quad (9)$$

with Liouvillian

$$L[j, k] = iH^{\text{inverse}}[\frac{\delta}{i\delta k} + \frac{1}{2}j, \frac{\delta}{i\delta j} - \frac{1}{2}k] - iH[\frac{\delta}{i\delta k} - \frac{1}{2}j, \frac{\delta}{i\delta j} + \frac{1}{2}k]. \quad (10)$$

It is interesting to restore powers of \hbar at this stage. We note that the terms with factors one-half come from the fundamental commutator and are of relative order \hbar . Expanding the r.h.s. in \hbar , the leading term cancels due to the relative minus sign in the summands in (10). The first non-vanishing contribution is linear in \hbar as the time derivative which also contains one \hbar . That contributions correspond to the classical limit of the Liouville equation.

$Z[j, k; t]$ is the generating functional of all equal-time correlators corresponding to Green functions at equal time. The generating functional of the connected correlators $W[j, k; t]$, however, is related to $Z[j, k; t]$ by

$$e^{W[j, k; t]} = Z[j, k; t]. \quad (11)$$

This relation implies for the r.h.s. of the Liouville equation

$$L[j, k]e^{W[j, k; t]} = \bar{L}[W][j, k; t]e^{W[j, k; t]} \quad (12)$$

which defines a non-linear evolution operator. The exponential also appears in the time derivative of the Liouville equation and thus cancels out. Evolution is now given by the Liouvillian-like equation

$$\partial_t W[j, k; t] = \bar{L}[W][j, k; t] \quad (13)$$

This equation qualitatively differs from the counterpart for $Z[j, k; t]$ since the operator \bar{L} is non-linear in its action on W .

In order to establish a relation to observables, we introduce the classical c-number field and momentum variables. We define the quantities

$$\varphi(t, \mathbf{x}) := \frac{\delta W[j, k; t]}{i\delta j(\mathbf{x})}, \quad \pi(t, \mathbf{x}) := \frac{\delta W[j, k; t]}{i\delta k(\mathbf{x})} \quad (14)$$

which coincide with the expectation values $\langle \Phi(\mathbf{x}) \rangle_t$ and $\langle \Pi(\mathbf{x}) \rangle_t$ when the currents vanish. We want to point out that the classical variables $\varphi(t, \mathbf{x})|_{j=k=0}$ and $\pi(t, \mathbf{x})|_{j=k=0}$ do depend on time and are independent of the picture chosen – in the opposite to their Schrödinger operator counterparts. In the definition (14), the classical field and momentum are functionals of the currents j, k . Suppose we can invert the relation and express the currents as functionals $j = j[\varphi, \pi]$, $k = k[\varphi, \pi]$, then the effective action defined by

$$\Gamma[\varphi, \pi; t] = \varphi(t) \cdot j + \pi(t) \cdot k + iW[j, k; t] \quad (15)$$

can be expressed as a functional of the classical variables. It obeys a relation dual to the definition (14)

$$\frac{\delta \Gamma[\varphi(t), \pi(t); t]}{\delta \varphi(t)} = j, \quad \frac{\delta \Gamma[\varphi(t), \pi(t); t]}{\delta \pi(t)} = k. \quad (16)$$

That implies that the currents vanish at the minimum of the effective action where the classical quantities have their interpretation as operator expectation values.

In order to apply terms correctly, let us remind the reader that the quantity Γ discussed here differs slightly from the definition used in standard field theory, namely, it corresponds to the generating functional of vertex functions at equal times. Here, the effective action itself has explicit time dependence from the classical fields, and an implicit one inferred from the evolution of the density matrix. The total time derivative thus behaves as $d\Gamma/dt = \dot{\varphi} \cdot \delta\Gamma/\delta\varphi + \dot{\pi} \cdot \delta\Gamma/\delta\pi + \partial_t\Gamma$, which, when compared with the time derivative of the definition (15), implies

$$\partial_t\Gamma[\varphi, \pi; t] = i\partial_t W[j, k; t] \quad (17)$$

where we took into account the time independence of the currents and the relation (16). It is now straight-forward to translate the equation of motion for the generating functional of the connected Green functions into an equation for Γ . One only has to express the Liouvillian in the evolution equation (13) in terms of φ and π . In $\bar{L}[W]$, currents can be replaced by the relations (16). The first derivatives of W are given in Eqs. (14), and higher derivatives can be found by successive differentiation of that relation. We get for the first few terms

$$\begin{aligned} -iW_{,jj} &= \varphi_{,j} = \Gamma_{,\varphi\varphi}^{-1} =: G^{(\varphi\varphi)} \\ -iW_{,jjj} &= -\Gamma_{,\varphi\varphi}^{-2} \left(\Gamma_{,\varphi\varphi\varphi} \Gamma_{,\varphi\varphi}^{-1} + \Gamma_{,\varphi\varphi\pi} \Gamma_{,\varphi\pi}^{-1} \right) \\ -iW_{,jk} &= \varphi_{,k} = \pi_{,j} = \Gamma_{,\varphi\pi}^{-1} =: G^{(\varphi\pi)} \\ -iW_{,jjk} &= -\Gamma_{,\varphi\varphi}^{-2} \left(\Gamma_{,\varphi\varphi\varphi} \Gamma_{,\varphi\pi}^{-1} + \Gamma_{,\varphi\varphi\pi} \Gamma_{,\pi\pi}^{-1} \right) \\ -iW_{,jkk} &= -\Gamma_{,\varphi\pi}^{-2} \left(\Gamma_{,\varphi\varphi\pi} \Gamma_{,\varphi\pi}^{-1} + \Gamma_{,\varphi\pi\pi} \Gamma_{,\pi\pi}^{-1} \right) \end{aligned} \quad (18)$$

where we wrote shorthand $\delta\Gamma/\delta\varphi =: \Gamma_{,\varphi}$ etc., and W itself has to be replaced by $-i(\Gamma - \varphi \cdot \Gamma_{,\varphi} - \pi \cdot \Gamma_{,\pi})$. Along that line of arguments, we can translate the operator $\bar{L}[W]$ and finally get the desired Liouville equation for the effective action, to wit

$$\partial_t\Gamma = F[\Gamma] = i \bar{L}[W] \big|_{j[\varphi,\pi], k[\varphi,\pi]}. \quad (19)$$

The classical limit of it was studied in [1] using a different approach. The relation (19) is local in the time parameter and the determining equation for Γ . Expanding the effective action in powers of φ and π

$$\begin{aligned} \Gamma[\varphi, \pi] &= \sum_{n=1}^{\infty} \frac{1}{n!} \left(\prod_{i=1}^n \int d^3\mathbf{x}_i \right) \times \\ &\quad \sum_{j=0}^n \Gamma_n^j(\mathbf{x}_1 \dots \mathbf{x}_n; t) \varphi(\mathbf{x}_1, t) \dots \varphi(\mathbf{x}_j, t) \pi(\mathbf{x}_{j+1}, t) \dots \pi(\mathbf{x}_n, t) \end{aligned} \quad (20)$$

and comparing the corresponding coefficients at both sides of (19), one gets an infinite non-linear and highly coupled hierarchy for the time dependence of the proper vertex functions Γ_n^j . The solution involves an infinite number of initial conditions

corresponding to the infinite set of observables necessary to describe a system completely. Suppose we can find a solution of that hierarchy, at least a perturbative one, one may ask for the time evolution of observables. We know that the c-number fields φ and π have their interpretation as expectation values of the position and momentum operator when the currents vanish. Thus, from the dual relation (16) we find the effective equations of motion

$$\frac{\delta\Gamma[\varphi(t), \pi(t); t]}{\delta\varphi(t)} = 0, \quad \frac{\delta\Gamma[\varphi(t), \pi(t); t]}{\delta\pi(t)} = 0. \quad (21)$$

as variational minimum of the effective action. These equations determine the time evolution of the average field $\langle\Phi\rangle_t$ and momentum $\langle\Pi\rangle_t$ resp. Expectation values of symmetrically ordered higher order operators are given by the derivatives of W in Eq. (18) evaluated at the solution of (21).

Scalar field

Let us consider the non-interacting motion of a scalar field characterized by the Hamiltonian

$$H^0 = \frac{1}{2} \int d^3x \left(\Pi^2 + \Phi(-\Delta + m^2)\Phi \right) \quad (22)$$

which, by Eq. (10), gives rise to the free Liouvillian

$$L^0 = i \int d^3x \left(j(\mathbf{x}) \frac{\delta}{i\delta k(\mathbf{x})} - k(\mathbf{x})(-\Delta + m^2) \frac{\delta}{i\delta j(\mathbf{x})} \right). \quad (23)$$

Since, in this simple case, the operator is even linear in the functional derivatives, its action on the exponential is also linear in W , $L^0 e^W = (L^0 W) e^W$. Rewriting everything in terms of the effective action yields

$$\partial_t \Gamma = F^0[\Gamma] = \int d^3x \left(\varphi(\mathbf{x})(-\Delta + m^2) \frac{\delta\Gamma}{\delta\pi(\mathbf{x})} - \pi(\mathbf{x}) \frac{\delta\Gamma}{\delta\varphi(\mathbf{x})} \right) \quad (24)$$

which has a remarkably homogeneity property. The r.h.s. is a map of the class of polynomials in φ and π of a given fixed order onto itself and the n-point vertices Γ_n in Eq. (20) obey a closed equation each. Time evolution can best be made explicit by a diagonalisation procedure using the normal coordinates ξ, ξ^*

$$\xi = \sqrt{\frac{\omega}{2}}\varphi + \frac{i}{\sqrt{2\omega}}\pi, \quad \omega_{\mathbf{k}} = \sqrt{m^2 + \mathbf{k}^2}, \quad (25)$$

where the expansion coefficients in (20) transform accordingly. The Liouville operator now takes the form

$$F^0[\Gamma] = i \int d^3k \omega \left(\xi \frac{\delta\Gamma[\xi, \xi^*]}{\delta\xi} - \xi^* \frac{\delta\Gamma[\xi, \xi^*]}{\delta\xi^*} \right) \quad (26)$$

which implies for time evolution (the index j now refers to the number of ξ 's in the expansion in normal coordinates)

$$\Gamma_n^{j\{\xi\}}(\mathbf{k}_1 \dots \mathbf{k}_n; t) = \Gamma_n^{j\{\xi\}}(\mathbf{k}_1 \dots \mathbf{k}_n; 0) \exp(i \sum_{i=1}^j \omega_{\mathbf{k}_i} t - i \sum_{i=j+1}^n \omega_{\mathbf{k}_i} t). \quad (27)$$

As expected, each proper mode just oscillates harmonically. We want to point out that motion is perfectly compatible with arbitrarily high order vertex functions, and there is no physical argument to neglect them in the first place. In that sense, in a non-interacting system higher correlation functions have to be taken into account in order to allow for general initial conditions.

In contrast to the simple form of the time evolution of the effective action, the solution of the on-shell conditions (21) involves to resolve a non-local non-linear equation for the classical fields φ and π even in the non-interacting theory.

The inclusion of a quartic interaction term $H = H^0 + \lambda \int d^3x \varphi^4$ modifies the Liouvillian by

$$L^{(\lambda)} = -i\lambda \int d^3x \left(4 \left(\frac{\delta}{i\delta j(\mathbf{x})} \right)^3 k(\mathbf{x}) + \frac{\delta}{i\delta j(\mathbf{x})} k^3(\mathbf{x}) \right). \quad (28)$$

This gives rise to the non-linear Liouvillian

$$\begin{aligned} F^\lambda[\Gamma] = & \lambda \int d^3x \left(4 \frac{\delta \Gamma}{\delta \pi(\mathbf{x})} \left[\int d^3u \int d^3v \int d^3w G^{(\varphi\varphi)}(\mathbf{x}, \mathbf{u}) G^{(\varphi\varphi)}(\mathbf{x}, \mathbf{v}) \times \right. \right. \\ & \left. \left[G^{(\varphi\varphi)}(\mathbf{x}, \mathbf{w}) \frac{\delta^3 \Gamma}{\delta \varphi(\mathbf{u}) \delta \varphi(\mathbf{v}) \delta \varphi(\mathbf{w})} + G^{(\varphi\pi)}(\mathbf{x}, \mathbf{w}) \frac{\delta^3 \Gamma}{\delta \varphi(\mathbf{u}) \delta \varphi(\mathbf{v}) \delta \pi(\mathbf{w})} \right] \right. \\ & \left. \left. - 3i\varphi(\mathbf{x}) G^{(\varphi\varphi)}(\mathbf{x}, \mathbf{x}) + \varphi^3(\mathbf{x}) \right] + \left(\frac{\delta \Gamma}{\delta \pi(\mathbf{x})} \right)^3 \varphi(\mathbf{x}) \right). \end{aligned} \quad (29)$$

The graphical representation of the complete time evolution including the free part is depicted in Fig. 1. The filled blob denotes the generating functional Γ , and full and dashed legs attached to it correspond to derivatives with respect to φ and π respectively. The unfilled circle with one leg stands for a factor φ and with two legs for the two-point correlators $G^{(\varphi\varphi)}$ and $G^{(\varphi\pi)}$. The diamond stands for the free kernel operator $-\Delta + m^2$ and the dashed circle for a factor π .

The first two graphs correspond to the classical non-interacting and the third through sixth graph to the classical interacting Liouvillian. Only the last graph is a quantum correction being of relative order \hbar^2 . The system can be expanded in powers of φ and π which leads to a hierarchy of coupled equations for the vertex functions Γ_n^j .

One may now start to attempt to solve the hierarchy for the vertex functions by cutting it at a certain order. However, this somehow pragmatic approach, however, is not guaranteed to yield a physically sensible result. Firstly, one runs into consistency problems with the hierarchy. Even worse, a check would require to calculate those terms which have been dropped in the cutting procedure in order to justify them to be neglected. Moreover, guided by the exact solution for the free case, where we



have already seen that higher correlators have to be treated at the same footing as all others, it is at first sight not evident why just the more complex dynamical structure should admit any such simplification. Secondly, cutting the hierarchy implicitly implies an assumption about the initial conditions for the higher vertex functions. It is not easy to see what physical initial preparation cutting the hierarchy and assuming particular initial values just for the lowest vertex functions represent. It is even more difficult to figure out what statistical assumptions about the system are hidden in a particular cutting procedure.

To summarize, the Liouville equation derived here makes a statement about the exact evolution of a system in mixed states. Any statement about the thermodynamic properties of that system, and in particular about how it approaches an equilibrium state cannot be read of from the dynamics but requires the application of the sophisticated tools of statistical mechanics. This goes beyond the scope of this letter and will be presented elsewhere.

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References

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$+4\lambda$ 
 $+4\lambda$ 

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